

Table1 Identification results of serum biomarkers in YHS group

NO	Rt	m/z determined	m/z calculated	Error (mDa)	Ion form	Molecular Formula	Metabolite Name	Trend	T'TEST
1	8.73	772.5930	771.5778	0.189	[M+H] ⁺	C ₄₃ H ₈₂ NO ₈ P	PC(15:0/20:2(11Z,14Z))	↓	1.594 × E ⁻³
2	0.60	130.0499	129.0426	0.486	[M+H] ⁺	C ₅ H ₇ NO ₃	Pyroglutamic acid	↓	1.654 × E ⁻²
3	2.20	249.1251	248.1161	2.912	[M+H] ⁺	C ₁₃ H ₁₆ N ₂ O ₃	6-Hydroxymelatonin	↑	4.540 × E ⁻⁵
4	6.25	546.3539	545.3481	-2.775	[M+H] ⁺	C ₂₈ H ₅₂ NO ₇ P	LysoPC(20:3(5Z,8Z,11Z))	↓	1.466 × E ⁻⁶
5	8.19	512.5064	511.4964	3.141	[M+H] ⁺	C ₃₂ H ₆₅ NO ₃	Cer(d18:0/14:0)	↓	6.952 × E ⁻⁹
6	8.78	719.5690	718.5536	-1.355	[M+H] ⁺	C ₄₇ H ₇₄ O ₅	DG(22:4(7Z,10Z,13Z,16Z)/22:5(4Z,7Z,10Z,13Z,16Z)/0:0)	↓	1.981 × E ⁻²
7	1.98	194.0794	193.0739	-0.035	[M+H] ⁺	C ₁₀ H ₁₁ NO ₃	Phenylacetyl glycine	↑	4.578 × E ⁻³
8	2.23	411.2492	410.2433	-3.366	[M+H] ⁺	C ₁₉ H ₃₉ O ₇ P	LPA(0:0/16:0)	↑	4.933 × E ⁻²
9	2.69	121.0649	120.0575	0.960	[M+H] ⁺	C ₈ H ₈ O	Phenylacetaldehyde	↑	4.446 × E ⁻³
10	3.06	136.0761	135.0684	2.714	[M+H] ⁺	C ₈ H ₉ NO	2-Phenylacetamide	↑	2.989 × E ⁻²
11	8.31	556.5300	555.5227	0.128	[M+H] ⁺	C ₃₄ H ₆₉ NO ₄	Cer(t18:0/16:0)	↑	5.923 × E ⁻³
12	8.89	770.5690	769.5622	-0.541	[M+H] ⁺	C ₄₃ H ₈₀ NO ₈ P	PC(15:0/20:3(5Z,8Z,11Z))	↓	1.618 × E ⁻²
13	2.25	758.5692	757.5622	-0.306	[M+H] ⁺	C ₄₂ H ₈₀ NO ₈ P	PC(14:0/20:2(11Z,14Z))	↑	3.516 × E ⁻³
14	5.46	224.0562	223.0481	3.917	[M+H] ⁺	C ₁₀ H ₉ NO ₅	4-(2-Amino-3-hydroxyphenyl)-2,4-dioxobutanoic acid	↑	2.124 × E ⁻⁷
15	6.99	538.3877	537.3794	1.885	[M+H] ⁺	C ₂₇ H ₅₆ NO ₇ P	LysoPE(0:0/22:0)	↓	1.504 × E ⁻²
16	1.72	209.0939	208.0848	-1.470	[M+H] ⁺	C ₁₀ H ₁₂ N ₂ O ₃	Formyl-5-hydroxykynurenamine	↑	3.473 × E ⁻⁴
17	2.32	185.0827	184.0736	2.899	[M+H] ⁺	C ₉ H ₁₂ O ₄	Vanylglycol	↑	2.157 × E ⁻³
18	8.34	802.6350	801.6248	4.570	[M+H] ⁺	C ₄₅ H ₈₈ NO ₈ P	PC(15:0/22:1(13Z))	↓	1.049 × E ⁻³
19	1.90	163.0383	164.0473	1.601	[M-H] ⁻	C ₉ H ₈ O ₃	Phenylpyruvic acid	↑	3.070 × E ⁻⁴

20	1.98	193.0349	194.0427	-2.627	[M-H]-	C ₆ H ₁₀ O ₇	D-Glucuronic acid	↑	4.211 × E ⁻²
21	8.49	790.5418	791.5465	3.185	[M-H]-	C ₄₅ H ₇₈ NO ₈ P	PC(15:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	↑	4.768 × E ⁻²
22	6.19	480.3096	481.3168	0.038	[M-H]-	C ₂₃ H ₄₈ NO ₇ P	LysoPC(15:0)	↓	1.101 × E ⁻²

↑ : YHS vs Control; ↓ : YHS vs Control

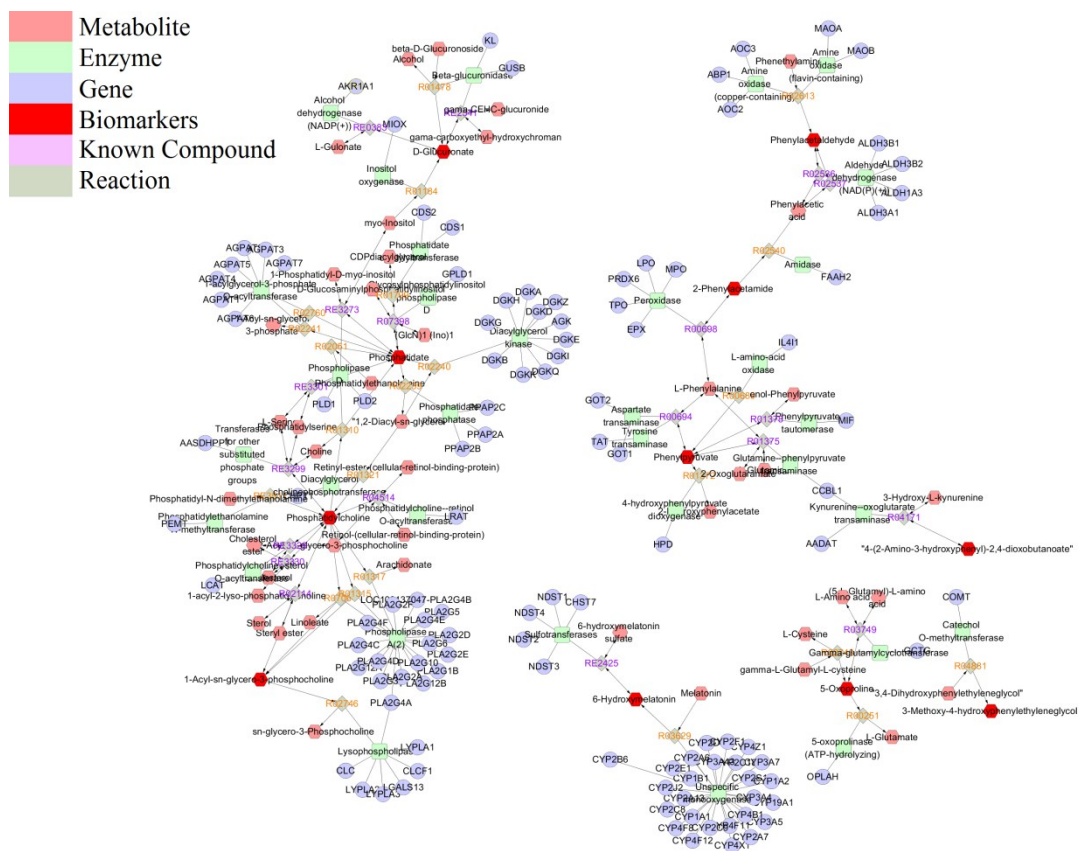


Fig. S1 Construction of the altered metabolic network associated YHS mice based on KEGG pathway database.